The Structure of the Vortex Liquid at the Surface of a Layered Superconductor

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Abstract

A density-functional approach is used to calculate the inhomogeneous vortex density distribution in the flux liquid phase at the planar surface of a layered superconductor, where the external magnetic field is perpendicular to the superconducting layers and parallel to the surface. The interactions with image vortices are treated within a mean field approximation as a *functional* of the vortex density. Near the freezing transition strong vortex density fluctuations are found to persist far into the bulk liquid. We also calculate the height of the Bean-Livingston surface barrier.

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Fluctuations of vortices in high-T_c superconductors give rise to a number of novel effects [1,2] the most prominent of which is probably the melting of the vortex lattice into a vortex liquid which was first proposed by Nelson [3] in 1988. While much work has been done to study the bulk properties of the vortex system, the influence of fluctuations on the behavior of flux vortices at the surface of a superconductor only rarely has been taken into account. Recently Brandt, Mints, and Snapiro [4] calculated the interaction of a single stack of thermally fluctuating pan-cake vortices with the planar surface of a layered superconductor. They found that fluctuations shift the short-range attraction between the vortices and their mirror-images to a long-range dipole-dipole interaction. In this Letter we consider a related problem, namely the interaction of a vortex-*liquid* with a planar surface.

In order to describe the vortex system in the liquid regime we will apply the density-functional theory of classical liquids [5]. The theory for the bulk vortex liquid has been worked out by Sengupta *et al.* [6] who have calculated bulk correlation functions and treated the freezing of the vortex liquid into the solid phase. In the present work we will compute the inhomogeneous density distribution of the vortices in front of a planar surface using the Wertheim-Lovett-Mou-Buff (WLMB) equation [7] together with a mean-field treatment of the image-forces. [8] The same method has recently successfully been applied in a different context, namely the structure of liquid water at a metallic interface [9]. From the equilibrium vortex-density profiles at the surface we calculate the local magnetic field which together with the image interactions determines the potential energy barrier [10] for pan-cake vortices entering into the sample. From this the location of the irreversibility line (IL) in the B-T-diagram is estimated for the case of zero bulk pinning and vanishing *geometrical* surface barrier [11].

Before discussing the surface problem we will shortly reconsider the density functional approach for the bulk vortex liquid following Sengupta *et al.* [6]. This enables us to compute the bulk direct correlation functions we need as input into the surface calculations described below. In the limit of zero interlayer Josephson coupling and for $\mathbf{H} \parallel \mathbf{c}$ the vortices in an N-layer superconductor can be viewed as a *two dimensional* classical system of N species of point particles interacting via the (asymptotically) logarithmic pair potential $V_n(r)$ of two vortices separated by n layers. In the limit $N \to \infty$ the Fourier transform of this pair potential is given by [12]

$$V(\mathbf{k}) = \frac{\epsilon_0 \lambda^2 \left[k_\perp^2 + (4/d^2)\sin^2(k_z d/2) \right]}{k_\perp^2 \left[1 + \lambda^2 k_\perp^2 + (4\lambda^2/d^2)\sin^2(k_z d/2) \right]}, \tag{1}$$

where $k_z (k_\perp)$ is the component of the wave-vector $\mathbf{k}$ perpendicular (parallel) to the layers. The parameter $\epsilon_0 = d\Phi_0^2/4\pi\lambda^2$ is the characteristic energy scale, β is the inverse temperature, $d \ll \lambda$ is the distance of the layers, and Φ_0 the flux quantum. The (2D-) pair potentials are repulsive for pancakes residing in the same layer and attractive but by the factor $(d/2\lambda)\exp(-nd/\lambda)$ weaker for pancakes in two separate layers of distance nd. However, the attractive and repulsive logarithmic potentials compensate each other on distances larger than λ leading to the usual short-range repulsion ($\sim K_0(r/\lambda)$) of Abrikosov vortices between two straight stacks of pancakes.

From the pair potentials $V_n(r)$ one can derive the liquid-state pair correlation functions $g_n(r)$ within standard liquid theory. As in Ref. [6] we use the hypernetted chain (HNC) approximation. The basic equations are then the Ornstein-Zernicke equation

$$h_n(r) = c_n(r) + \varrho_B \sum_m \int d^2\mathbf{r}' h_m(r') c_{n-m}(|\mathbf{r} - \mathbf{r}'|) \tag{2}$$

and the HNC-closure relation

$$g_n(r) = \exp\left[-\beta V_n(r) + h_n(r) - c_n(r)\right] \tag{3}$$

for the total correlation function $h_n(r) = g_n(r) - 1$ and the direct correlation function $c_n(r)$, where ϱ_B is the bulk density of the vortex liquid. For the numerical (iterative) solution of these equations it is appropriate to reformulate Eq. (2) in $\mathbf{k}$-space and to separate the direct correlation function $c_n(r)$ into a long-range and a short-range part. (Note that $c_n(r) \to -\beta V_n(r)$ as $r \to \infty$.) We were able to obtain self consistent solutions of the complete set of Eqs. (2) and (3) for a periodic system with 512 layers using a Fast Hankel transform method [13].

The phase boundary between the vortex liquid and the vortex solid was obtained in a different way than in Ref. [6] namely by examining the thermodynamical stability of the system, i.e. we looked at the spinodal curve rather than the coexistence line at the first order phase transition. The system becomes unstable if the second functional derivative of the grand canonical potential w.r.t. the density, $\mathcal{M}(\mathbf{r}, z, \mathbf{r}', z') = \delta^2\Omega/\delta\varrho(\mathbf{r}, z)\delta\varrho(\mathbf{r}', z')$, is no longer positiv definite. [14] In the case considered here $\mathcal{M}(\mathbf{r}, z, \mathbf{r}', z')$ is diagonal in $\mathbf{k}$-space because of the translational invariance of the vortex-system in all three space directions, $\mathcal{M}(\mathbf{k}, \mathbf{k}') = (1 - c(k_z, k_\perp))\delta(\mathbf{k} - \mathbf{k}')$. As expected, near the spinodal curve the system becomes unstable w.r.t. to fluctuations of the density $\sim e^{i\mathbf{k}_\perp \mathbf{r}}$ with $|\mathbf{k}_\perp| \approx 2\pi\varrho_B^{1/2}$ ($k_z = 0$), which indicates that the formation of a vortex lattice becomes favorable. The freezing line (spinodal curve) in the (B,T)-diagram is then obtained by extrapolating $1 - c(k_z, k_\perp)$ to zero. For high magnetic fields B the transition temperature approaches the 2D-melting temperature T_{2D} which is independent of the vortex density [6].

We now turn to the calculation of the local vortex density near the surface of the superconductor. We start with the Wertheim-Lovett-Mou-Buff (WLMB) equation [7] which is an exact relation following from classical density-functional theory. In a more general context this system of integro-differential equations relates the particle densities ϱ_α of species α to an external potential V_α:

$$\nabla_1 \log \varrho_\alpha(1) = -\beta\nabla_1 V_\alpha(1) + \sum_\beta \int d2 \nabla_2 \varrho_\beta(2) c_{\alpha\beta}(1, 2, [\varrho]) \tag{4}$$

Here, $c_{\alpha\beta}(1, 2, [\varrho])$ is the *inhomogeneous* direct correlation function which is a functional of the density itself. In the following we will again work in the HNC approximation and replace $c_{\alpha\beta}(1, 2, [\varrho])$ by its bulk version. We introduce a cartesean coordinate system where the (y,z)-plane is the surface of the superconductor which fills the half-space at $x > 0$. Because of the translational invariance in z-direction we are left with one equation for the vortex density $\varrho(x)$ in each layer which is a function of x only. Now, the bulk direct correlation function $c_n(r)$ is written as a sum of a long-range and a short-range part, $c_n(r) = c_n^{SR}(r) - \beta V_n(r)$, we carry out the integration parallel to the surface, and define

$$c^{SR,\|}(x) = \sum_n \int_x^\infty \frac{2r\,dr}{\sqrt{r^2 - x^2}} c_n^{SR}(r).$$

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With $\sum_n V_n(r) = (\epsilon_0/2\pi)K_0(r/\lambda)$ the WLMB-equation (4) then becomes

$$\frac{d}{dx}\log\varrho(x) = \beta\Delta\varrho\lambda\epsilon_0 e^{-x/\lambda} + \beta F^I(x,[\varrho]) + \int\limits_0^\infty dx'\frac{d\varrho}{dx'}c^{SR,\|}(|x-x'|) - \frac{\beta\epsilon_0\lambda}{2}\int\limits_0^\infty dx'\frac{d\varrho}{dx'}e^{-|x-x'|/\lambda}.$$

(5)

Eq. (5) is the basis for our numerical calculation. The first term on the r.h.s. of Eq. (5) gives the force produced by an exponentially decaying shielding current at the surface of the superconductor which arises from the homogeneous solution of the London equation. The second term is the image force which is the sum of the self-image force F^{SI} and the force F^{OI} produced by the images of all other pancakes, $F^I(x,[\varrho]) = F^{SI}(x) + F^{OI}(x,[\varrho])$. The third term in Eq. (5) gives the mean force caused by the liquid correlations and the last term represents the electromagnetic vortex-vortex interaction.

Eq. (5) has to be solved for the density $\varrho(x)$ at $x > 0$ with $\varrho(x) \overset{x\to\infty}{\Longrightarrow} \varrho_B$ while the parameter $\Delta\varrho$ is determined by the condition that the *potential of mean force*, $V_{\mathrm{PMF}}(x) = -k_BT\ln(\varrho(x)/\varrho_B)$ is zero at the surface ($\varrho(0) = \varrho_B$). The local magnetic field $B(x)$ then reads

$$B(x) = \Phi_0(\Delta\varrho - \varrho_B)e^{-x/\lambda} + \frac{\Phi_0}{2\lambda}\int\limits_0^\infty \varrho(x')e^{-|x'-x|/\lambda}dx',$$

(6)

the applied field is $B_a = B(0)$, and the bulk magnetic field is given by $B_0 = B(\infty) = \varrho_B\Phi_0$.

In the following we will derive an expression for the image forces F^I within a mean field approximation. The self image force acting on a pancake vortex at position $\mathbf{r} = (x,0)$ is given by

$$F^{SI}(x) = -\frac{\epsilon_0}{4\pi x} \quad (x > \xi),$$

(7)

where the cut-off ξ is related to the coherence length. The x-component of the force exerted on the same vortex by the image of a second vortex located at $\mathbf{r}'$ in layer n is

$$f_n(\mathbf{r},\mathbf{r}') = \frac{V_n'\left(\sqrt{r_{12}^2 + 4xx'}\right)(x+x')}{\sqrt{r_{12}^2 + 4xx'}}$$

with $r_{12} = |\mathbf{r} - \mathbf{r}'|$. Thus, the average total force produced by the non-self images can be written

$$F^{OI}(x,[\varrho]) = \sum_n \int f_n(\mathbf{r},\mathbf{r}')\varrho(\mathbf{r}')h_n(\mathbf{r}'|\mathbf{r})d\mathbf{r}'$$

(8)

where $h_n(\mathbf{r}'|\mathbf{r})$ is the total correlation function for the inhomogeneous liquid distribution at the surface. Here we assume that forces *parallel* to the surface cancel each other on the average. If the total correlation function $h_n(\mathbf{r}'|\mathbf{r})$ is again approximated by its bulk version $h_n(r_{12})$ the non-self image force F^{OI} can finally be expressed as a *linear functional* of the vortex density $\varrho(x)$,

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$$F^{OI}(x, [\varrho]) = \int_0^\infty \varrho(x')\mathcal{J}(x, x')dx'. \tag{9}$$

The kernel $\mathcal{J}(x, x')$ is given by

$$\mathcal{J}(x, x') = (x + x') \sum_n \int_{|x-x'|}^\infty \frac{2r_{12}h_n(r_{12})V_n'\left(\sqrt{r_{12}^2 + 4xx'}\right)}{\sqrt{r_{12}^2 - (x - x')^2}\sqrt{r_{12}^2 + 4xx'}}dr_{12}. \tag{10}$$

It is important to notice that the force of the non-self images cancels the long-range self-image force for sufficient large x. Indeed, writing $V_n(x) \sim q_n \ln(x/\xi)$ for $x > \lambda$ with 'charges' $q_0 = -1$, $q_{n\neq 0} \approx (d/2\lambda)e^{-nd/\lambda}$ ($\sum_n q_n = 0$), setting $\varrho(x) = \varrho_B$, and using the 'screening condition' for the total correlation function $h_n(r)$, $q_0 + \sum_n \int d^2\mathbf{r} \varrho_B q_n h_n(r) = 0$, one can perform the integrals (9) and (10) analytically and gets $F^{OI} \xrightarrow{x\to\infty} \epsilon_0/4\pi x = -F^{SI}$.

In what follows we present results of the numerical solution of Eq. (5). We introduce the dimensionless parameters $f = \lambda^2\varrho_B$, $\Gamma = \beta\epsilon_0$, $\delta = d/\lambda$, and $\kappa = \lambda/\xi$. All calculations have been performed for $\kappa = 100$ and $\delta = 0.01$ while f and Γ were varied. About 10^4 iterations of Eq. (5) on a grid of 2048 sites were needed to achieve convergence. However, when approaching the freezing transition of the vortex liquid the rate of convergence becomes slower and the numerical procedure finally diverges. The kernel $\mathcal{J}(x, x')$ for the image-forces (Eq. (10)) can be calculated once and then stored in a lookup-table.

Fig. 1 shows the so-obtained vortex density profiles for $f = 0.75$ and parameters $\Gamma = 100$, 250, and 360. Freezing occurs at approximately $\Gamma = 380$. It is seen that near the freezing transition strong density fluctuations persist far into the bulk liquid, so that the vortex-liquid is still solid-like at the surface. These fluctuations are washed out at higher temperatures (lower values of Γ). The corresponding magnetic field near the surface is shown in the left-hand inset of Fig. 1. Directly at the surface (invisible in Fig. 1) the density rapidly drops from ϱ_B to almost zero, which reflects the existence of a Bean-Livingston surface barrier [10]. This surface barrier is shown in the right-hand inset of Fig. 1 where the potential of mean force V_{PMF} is plotted for several values of the parameter $f = 0.6, 0.75, 1.0, 2.0$ and $\Gamma = 250$. The barrier height U turns out to be nearly independent of the temperature but decreases with increasing magnetic field (parameter f). This is shown in the inset of Fig. 2.

When the applied field is increased above its equilibrium value vortices will start to enter into the sample, where the flux-entry rate $\mathcal{R}$ is determined by the Boltzmann factor $e^{-\beta U}$. The irreversibility line (IL) separates the irreversible and the reversible part of the phase diagram on experimental time scales and is thus given by $\mathcal{R} = const$. We can therefore estimate (up to a constant factor) the location of the surface-barrier induced IL in the B-T-diagram by the condition $U(B) = ak_BT$, where a is a constant.

In order to compare with experimental results we will in the following use typical parameters for $Bi_2Sr_2CaCu_2O_8$ (BSCCO). The London penetration depth is taken to have a temperature dependence $\lambda(T) = \lambda(0)(1 - (T/T_C)^4)^{1/2}$ with $\lambda(0) = 1400$ Å and $T_C = 93$ K, $\kappa = 100$, and $d = 15$ Å. Fig. 2 (broken line) shows the melting line (spinodal curve) of the flux-line lattice in BSCCO as obtained by the method described above. For $T \gtrsim 50$ K it agrees well with the experimental data of Majer et $al.$ [11] ($\diamond$) . Deviations at low temperatures are possibly an effect of the Josephson interaction which has not been taken into account here. Fig. 2 (solid line) also shows the estimated location of the IL. A constant

factor $a = 42$ was chosen such that the curve lies near the experimentally obtained IL ($+$) from Ref. [11] for a sample of triangular cross-section, where the geometrical surface barrier is absent. Since bulk pinning plays no role in these experiments either, as argued in Ref. [11], the IL shown in Fig. 2 originates from a *Bean-Livingston* surface barrier alone. Though our simple calculation may not be applicable to this experiment in detail because of the more complicated sample geometry and possible effects of the surface roughness, the qualitative features of the IL found here are the same as those found in the experiment. In both cases the IL has a negative slope dB/dT and is much steeper than the melting line crossing the latter one at some point.

In conclusion we have calculated the density distribution of pan-cake vortices in the flux liquid phase at the surface of a layered superconductor using density functional theory and a mean field treatment of the image-interactions. Near the melting line strong density fluctuations are found to reach far into the bulk liquid. This could possibly enhance bulk-pinning near the surface. It is shown that a Bean-Livingston barrier exists from which we estimate the location of the irreversibility line (IL) in the B-T-plane which is qualitatively consistent with experimental findings for BSCCO crystals.
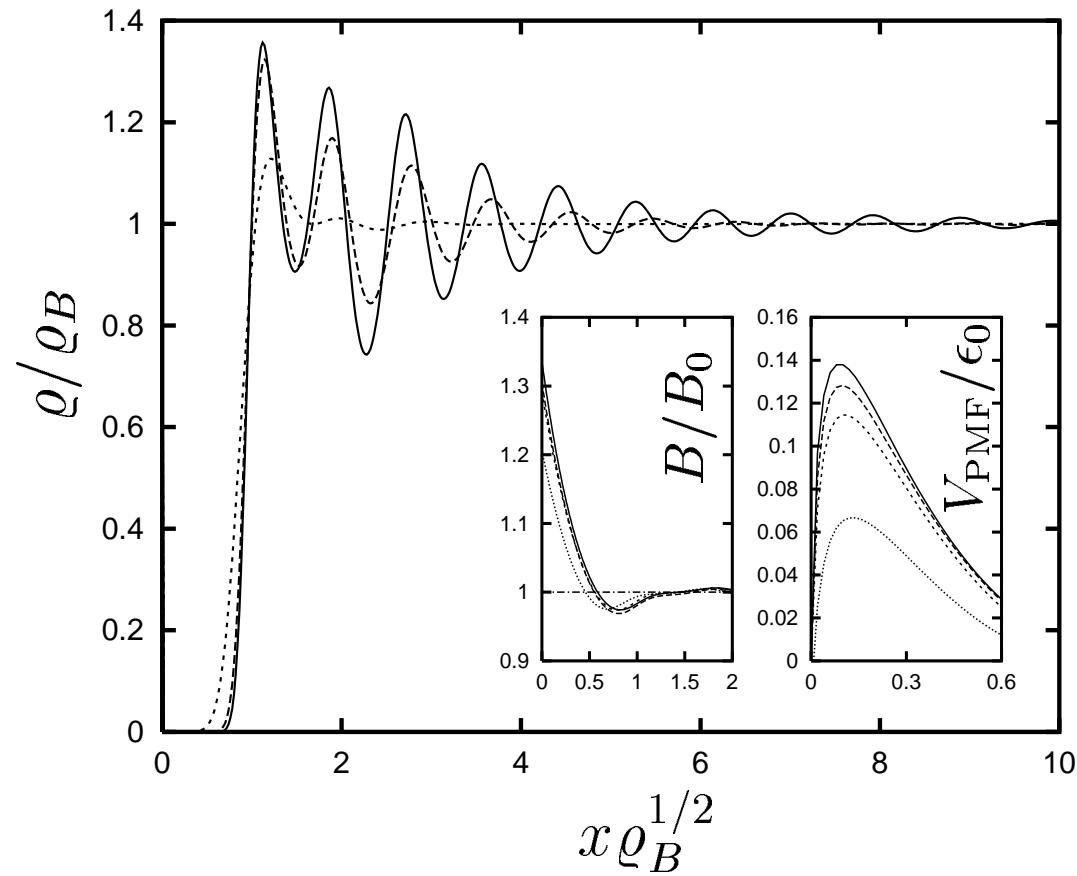
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FIGURES

FIG. 1. Density profile $\varrho(x)$ for constant bulk density ($f = 0.75$) and different temperatures ($\Gamma = 100$, 250, and 360). The right-hand inset shows the potential of mean force (PMF) at constant temperature ($\Gamma = 250$) for different bulk densities ($f = 0.6, 0.75, 1.0, 2.0$, from the upper to the lower curve). The left-hand inset gives the internal magnetic field $B(x)$ at the surface for the same set of parameters.

FIG. 2. The melting line of the vortex lattice in $Bi_2Sr_2CaCu_2O_8$: Experimental data from Ref. [11] ($\diamond$) and this work (dashed line). Irreversibility line (IL): Experimental data for a sample with triangular cross-section from Ref. [11] ($+$) and as estimated in this work (solid line, see text). The inset shows the barrier height U/ϵ_0 as function of f.